



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 25, 2024 – 06:16 AM EDT

PDB ID : 5TS1  
Title : Crystal structure of MHC-I H2-KD complexed with peptides of Mycobacterial tuberculosis (YYQSGLSIV)  
Authors : Jiang, J.; Natarajan, K.; Margulies, D.  
Deposited on : 2016-10-27  
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.37.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

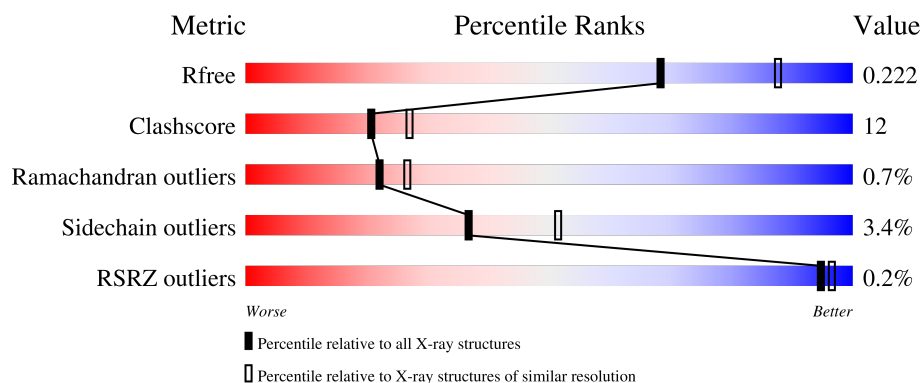
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*





The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	275	 67% 30% ..
1	C	275	 72% 25% ..
1	E	275	 72% 26% ..
1	G	275	 69% 28% ..
2	B	100	 69% 28% .

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Mol	Chain	Length	Quality of chain
2	D	100	 77% 21% •
2	F	100	 73% 24% •
2	H	100	 79% 19% •
3	P	9	 89% 11%
3	Q	9	 67% 33%
3	R	9	 78% 22%
3	S	9	 44% 44% 11%

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13146 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called H-2 class I histocompatibility antigen, K-D alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			2245	1422	401	415	7			
1	C	273	Total	C	N	O	S	0	0	0
			2251	1428	401	415	7			
1	E	273	Total	C	N	O	S	0	0	0
			2252	1428	401	416	7			
1	G	273	Total	C	N	O	S	0	0	0
			2251	1428	401	415	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	114	HIS	GLN	conflict	UNP P01902
A	276	PRO	LEU	conflict	UNP P01902
C	114	HIS	GLN	conflict	UNP P01902
C	276	PRO	LEU	conflict	UNP P01902
E	114	HIS	GLN	conflict	UNP P01902
E	276	PRO	LEU	conflict	UNP P01902
G	114	HIS	GLN	conflict	UNP P01902
G	276	PRO	LEU	conflict	UNP P01902

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			833	531	141	158	3			
2	D	100	Total	C	N	O	S	0	0	0
			833	531	141	158	3			
2	F	100	Total	C	N	O	S	0	0	0
			833	531	141	158	3			
2	H	100	Total	C	N	O	S	0	0	0
			836	533	141	158	4			

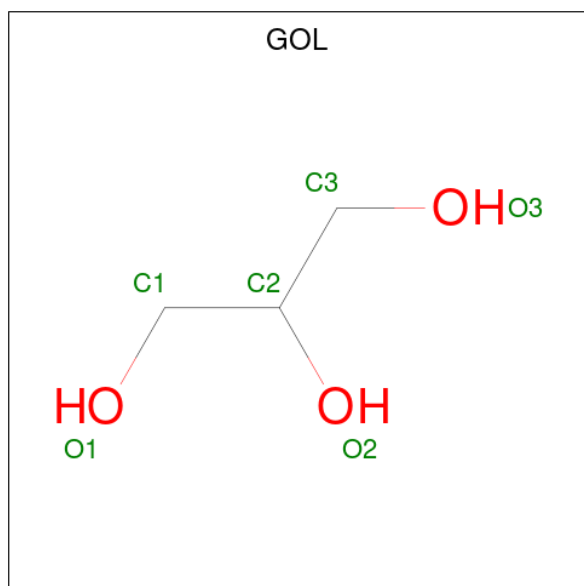
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
D	0	MET	-	initiating methionine	UNP P61769
F	0	MET	-	initiating methionine	UNP P61769
H	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called Peptide (P9) of Mtb85B (Mycobacterium tuberculosis) YYQS-GLSIV.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	P	9	Total	C	N	O	0	0	0
			73	48	10	15			
3	Q	9	Total	C	N	O	0	0	0
			73	48	10	15			
3	R	9	Total	C	N	O	0	0	0
			73	48	10	15			
3	S	9	Total	C	N	O	0	0	0
			73	48	10	15			

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



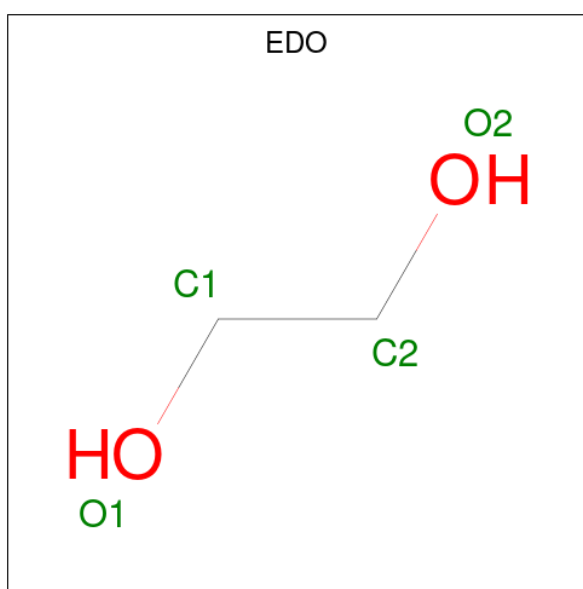
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	92	Total	O	0	0
			92	92		
6	B	27	Total	O	0	0
			27	27		

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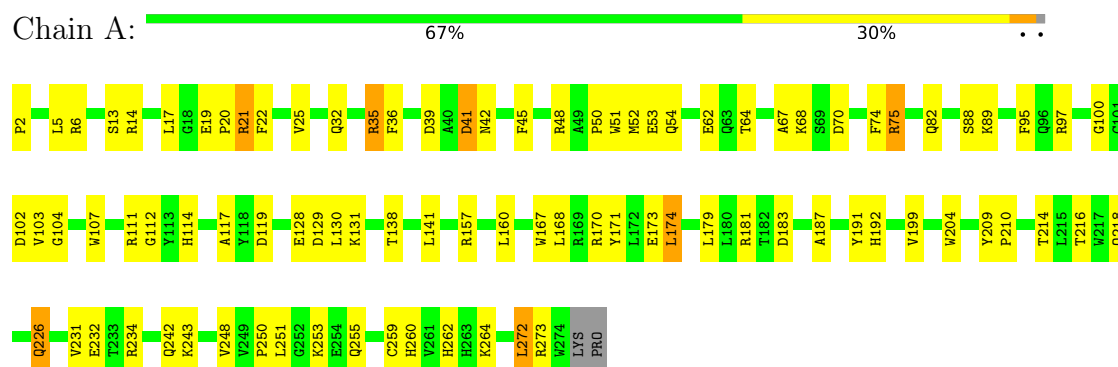
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	P	2	Total 2	O 2	0	0
6	C	88	Total 88	O 88	0	0
6	D	32	Total 32	O 32	0	0
6	Q	3	Total 3	O 3	0	0
6	E	79	Total 79	O 79	0	0
6	F	27	Total 27	O 27	0	0
6	R	1	Total 1	O 1	0	0
6	G	93	Total 93	O 93	0	0
6	H	24	Total 24	O 24	0	0
6	S	4	Total 4	O 4	0	0

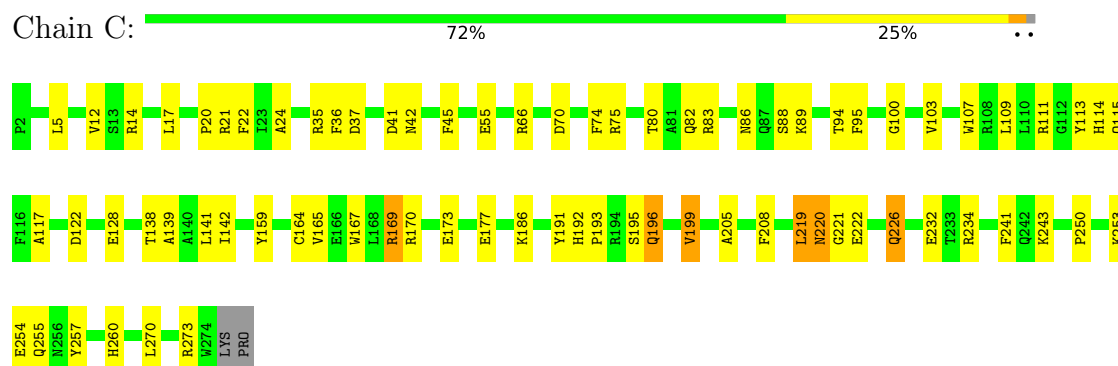
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

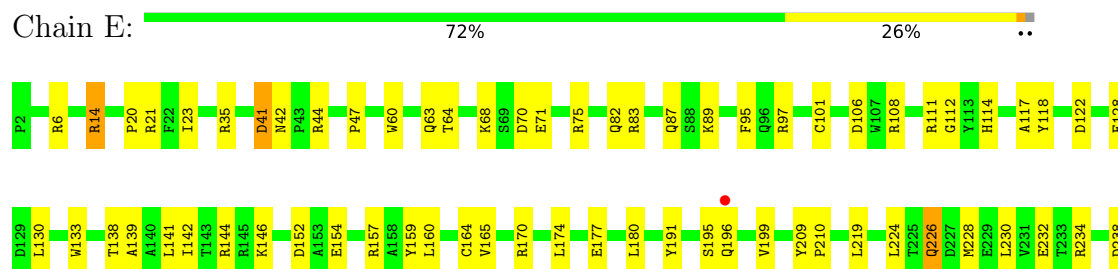
- Molecule 1: H-2 class I histocompatibility antigen, K-D alpha chain



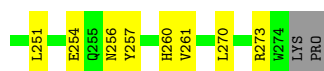
- Molecule 1: H-2 class I histocompatibility antigen, K-D alpha chain



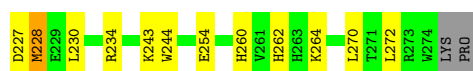
- Molecule 1: H-2 class I histocompatibility antigen, K-D alpha chain







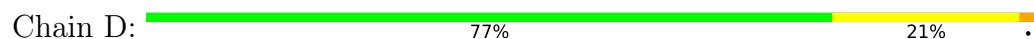
- Molecule 1: H-2 class I histocompatibility antigen, K-D alpha chain



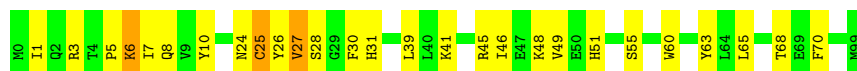
- Molecule 2: Beta-2-microglobulin



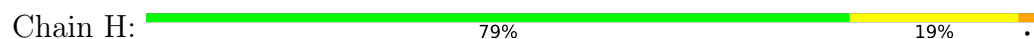
- Molecule 2: Beta-2-microglobulin



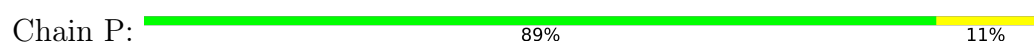
- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin



- Molecule 3: Peptide (P9) of Mtb85B (Mycobacterium tuberculosis) YYQSGLSIV

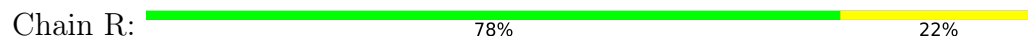




- Molecule 3: Peptide (P9) of Mtb85B (Mycobacterium tuberculosis) YYQSGLSIV



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- Molecule 3: Peptide (P9) of Mtb85B (Mycobacterium tuberculosis) YYQSGLSIV



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	47.30Å 88.96Å 109.95Å 89.97° 93.83° 90.04°	Depositor
Resolution (Å)	47.20 – 2.30 47.20 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.2 (47.20-2.30) 98.0 (47.20-2.30)	Depositor EDS
$R_{merge}$	0.23	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.43 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, $R_{free}$	0.187 , 0.224 0.190 , 0.222	Depositor DCC
$R_{free}$ test set	3903 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.7	Xtriage
Anisotropy	0.602	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 21.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.450 for -h,k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13146	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.77% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, EDO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.42	1/2314 (0.0%)	0.70	3/3149 (0.1%)
1	C	0.40	0/2320	0.71	2/3157 (0.1%)
1	E	0.38	0/2321	0.69	0/3158
1	G	0.59	4/2320 (0.2%)	0.70	0/3157
2	B	0.41	0/856	0.69	0/1159
2	D	0.34	0/856	0.69	0/1159
2	F	0.40	1/856 (0.1%)	0.65	0/1159
2	H	0.35	0/859	0.68	2/1162 (0.2%)
3	P	0.44	0/74	0.55	0/98
3	Q	0.35	0/74	0.74	0/98
3	R	0.44	0/74	0.54	0/98
3	S	0.44	0/74	0.91	1/98 (1.0%)
All	All	0.44	6/12998 (0.0%)	0.70	8/17652 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	E	0	1
All	All	0	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	35	ARG	NE-CZ	-12.38	1.17	1.33
1	G	35	ARG	CZ-NH1	-11.47	1.18	1.33
1	G	35	ARG	CZ-NH2	-9.83	1.20	1.33
1	G	35	ARG	CD-NE	-8.70	1.31	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	75	ARG	NE-CZ	-5.25	1.26	1.33
2	F	25	CYS	CB-SG	-5.21	1.73	1.81

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	174	LEU	CA-CB-CG	7.03	131.47	115.30
2	H	65	LEU	CA-CB-CG	6.51	130.28	115.30
1	A	251	LEU	CA-CB-CG	6.03	129.16	115.30
2	H	80	CYS	CA-CB-SG	5.30	123.55	114.00
1	C	219	LEU	CA-CB-CG	5.28	127.44	115.30
1	C	169	ARG	NE-CZ-NH1	-5.22	117.69	120.30
3	S	6	LEU	CA-CB-CG	5.05	126.91	115.30
1	A	272	LEU	CB-CG-CD2	-5.01	102.49	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	226	GLN	Peptide
1	E	195	SER	Peptide

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2245	0	2095	66	1
1	C	2251	0	2113	64	0
1	E	2252	0	2110	60	1
1	G	2251	0	2113	65	0
2	B	833	0	796	22	1
2	D	833	0	796	18	0
2	F	833	0	796	22	1
2	H	836	0	803	16	0
3	P	73	0	72	2	0
3	Q	73	0	72	2	0
3	R	73	0	72	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	S	73	0	72	5	0
4	A	12	0	16	0	0
4	D	6	0	8	0	0
4	F	6	0	8	0	0
4	G	6	0	8	0	0
4	H	6	0	8	0	0
5	A	4	0	6	0	0
5	C	8	0	12	2	0
6	A	92	0	0	8	2
6	B	27	0	0	1	0
6	C	88	0	0	7	1
6	D	32	0	0	0	0
6	E	79	0	0	13	2
6	F	27	0	0	1	0
6	G	93	0	0	5	1
6	H	24	0	0	0	0
6	P	2	0	0	0	0
6	Q	3	0	0	0	0
6	R	1	0	0	0	0
6	S	4	0	0	2	0
All	All	13146	0	11976	302	5

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (302) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:130:LEU:O	1:E:157:ARG:NH2	1.80	1.14
1:A:255:GLN:O	1:A:273:ARG:NH1	2.00	0.95
1:G:97:ARG:HE	1:G:114:HIS:HE1	1.14	0.91
1:E:101:CYS:SG	6:E:325:HOH:O	2.30	0.88
1:G:220:ASN:O	1:G:222:GLU:N	2.07	0.87
1:G:216:THR:HG21	1:G:224:LEU:HD22	1.55	0.86
1:G:20:PRO:HG2	1:G:75:ARG:HG2	1.59	0.85
1:E:42:ASN:OD1	1:E:44:ARG:NH1	2.13	0.81
1:C:20:PRO:HG2	1:C:75:ARG:HG2	1.63	0.79
1:A:128:GLU:OE1	6:A:401:HOH:O	2.00	0.79
1:E:122:ASP:OD1	2:F:60:TRP:NE1	2.15	0.77
1:G:97:ARG:HE	1:G:114:HIS:CE1	2.01	0.77
1:G:138:THR:HA	1:G:141:LEU:HD12	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:130:LEU:O	1:G:157:ARG:NH2	2.18	0.77
1:E:273:ARG:NH1	6:E:303:HOH:O	2.17	0.76
1:E:138:THR:HA	1:E:141:LEU:HD12	1.68	0.74
1:A:97:ARG:HE	1:A:114:HIS:CE1	2.05	0.74
1:E:164:CYS:SG	6:E:302:HOH:O	2.45	0.73
1:E:154:GLU:OE2	6:E:301:HOH:O	2.07	0.73
1:C:232:GLU:OE1	2:D:28:SER:OG	2.06	0.73
1:A:97:ARG:HE	1:A:114:HIS:HE1	1.35	0.72
1:G:14:ARG:HB2	1:G:17:LEU:HB2	1.71	0.72
1:G:66:ARG:O	6:G:401:HOH:O	2.08	0.71
1:C:21:ARG:HH21	1:C:37:ASP:CG	1.92	0.71
2:D:25:CYS:HB2	2:D:39:LEU:HD21	1.73	0.71
1:G:97:ARG:NE	1:G:114:HIS:HE1	1.87	0.71
1:A:130:LEU:O	1:A:157:ARG:NH2	2.23	0.70
1:C:186:LYS:O	6:C:401:HOH:O	2.09	0.70
1:A:138:THR:HA	1:A:141:LEU:HD12	1.73	0.70
2:B:98:ASP:OD1	2:B:98:ASP:N	2.24	0.70
1:C:205:ALA:O	6:C:402:HOH:O	2.10	0.70
1:E:20:PRO:HG2	1:E:75:ARG:HG2	1.73	0.70
1:E:154:GLU:OE2	1:E:157:ARG:NH1	2.24	0.70
1:G:106:ASP:OD1	1:G:108:ARG:N	2.25	0.69
1:G:111:ARG:HD2	1:G:128:GLU:HG3	1.74	0.69
1:E:6:ARG:NH2	6:E:305:HOH:O	2.25	0.68
1:A:97:ARG:NE	1:A:114:HIS:HE1	1.91	0.68
1:C:21:ARG:NH2	1:C:37:ASP:OD1	2.18	0.67
1:E:106:ASP:OD1	1:E:108:ARG:HB2	1.95	0.66
1:C:220:ASN:O	1:C:222:GLU:N	2.28	0.66
1:G:226:GLN:O	6:G:402:HOH:O	2.13	0.66
1:G:226:GLN:C	1:G:228:MET:H	1.98	0.66
1:A:52:MET:SD	6:A:436:HOH:O	2.53	0.65
1:C:219:LEU:HD22	1:C:220:ASN:H	1.60	0.65
1:G:214:THR:HB	1:G:262:HIS:HB2	1.77	0.65
1:C:138:THR:HA	1:C:141:LEU:HD12	1.79	0.64
1:G:66:ARG:NH2	3:S:2:TYR:O	2.28	0.64
1:E:139:ALA:HA	1:E:142:ILE:HD12	1.80	0.64
1:A:41:ASP:OD1	1:A:42:ASN:N	2.30	0.64
1:E:21:ARG:HE	1:E:23:ILE:HD11	1.62	0.64
2:F:25:CYS:HB2	2:F:39:LEU:HD21	1.80	0.63
1:E:111:ARG:HG3	1:E:112:GLY:N	2.11	0.63
1:G:212:ASP:OD2	1:G:264:LYS:NZ	2.32	0.63
1:C:117:ALA:HB2	2:D:60:TRP:CD2	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:170:ARG:O	1:E:174:LEU:HD22	1.99	0.62
1:G:218:GLN:HE21	1:G:224:LEU:HD23	1.64	0.61
1:E:191:TYR:HE2	1:E:254:GLU:HG2	1.65	0.61
1:A:111:ARG:NH2	6:A:407:HOH:O	2.32	0.61
1:C:24:ALA:O	6:C:403:HOH:O	2.16	0.61
1:E:60:TRP:HA	6:E:364:HOH:O	2.00	0.61
1:G:109:LEU:HD12	1:G:161:GLU:HA	1.83	0.61
1:C:169:ARG:O	1:C:173:GLU:HG3	2.01	0.60
2:H:9:VAL:HG22	2:H:80:CYS:SG	2.42	0.60
1:A:214:THR:HB	1:A:262:HIS:HB2	1.83	0.59
2:F:7:ILE:HG12	2:F:27:VAL:HG23	1.83	0.59
1:C:191:TYR:HE2	1:C:254:GLU:HG2	1.67	0.59
1:A:5:LEU:HB2	1:A:168:LEU:HD13	1.84	0.59
1:A:82:GLN:OE1	1:A:89:LYS:HD3	2.04	0.58
1:E:191:TYR:CE2	1:E:254:GLU:HG2	2.38	0.58
1:C:250:PRO:HB2	1:C:253:LYS:HD2	1.84	0.58
1:E:226:GLN:NE2	6:E:307:HOH:O	2.29	0.58
2:F:27:VAL:HG13	2:F:30:PHE:CE1	2.38	0.58
1:C:220:ASN:C	1:C:222:GLU:H	2.07	0.58
2:B:1:ILE:HD13	2:B:3:ARG:HE	1.69	0.57
1:G:35:ARG:NH2	1:G:37:ASP:HB3	2.19	0.57
1:A:170:ARG:O	1:A:174:LEU:HD22	2.05	0.57
1:G:42:ASN:O	6:G:403:HOH:O	2.17	0.57
1:E:83:ARG:NH2	6:E:309:HOH:O	2.37	0.56
1:C:88:SER:O	6:C:404:HOH:O	2.17	0.56
1:C:111:ARG:HH11	1:C:128:GLU:HG3	1.69	0.56
1:C:122:ASP:OD1	2:D:60:TRP:NE1	2.21	0.56
1:C:192:HIS:NE2	2:D:98:ASP:OD2	2.38	0.56
1:A:272:LEU:HB2	6:A:403:HOH:O	2.05	0.56
1:E:159:TYR:OH	6:E:302:HOH:O	2.16	0.56
1:C:219:LEU:HD13	1:C:220:ASN:HB2	1.88	0.55
1:E:133:TRP:HB2	1:E:144:ARG:HG3	1.88	0.55
1:G:244:TRP:CE2	2:H:99:MET:HE1	2.42	0.55
1:E:196:GLN:HB2	6:E:375:HOH:O	2.06	0.55
1:C:117:ALA:HB2	2:D:60:TRP:CE2	2.41	0.55
2:H:58:LYS:N	2:H:58:LYS:HD3	2.21	0.55
1:A:218:GLN:HG3	1:A:260:HIS:CE1	2.41	0.55
1:E:41:ASP:OD2	1:E:44:ARG:NH1	2.40	0.55
1:G:35:ARG:NH2	1:G:37:ASP:CB	2.69	0.55
2:F:5:PRO:HB2	2:F:27:VAL:HG22	1.89	0.54
1:E:87:GLN:OE1	1:E:118:TYR:OH	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:ASP:OD1	1:C:42:ASN:N	2.35	0.54
1:C:139:ALA:HA	1:C:142:ILE:HD12	1.90	0.54
1:G:171:TYR:OH	3:S:1:TYR:N	2.36	0.53
2:B:70:PHE:CZ	2:B:72:PRO:HG3	2.44	0.53
2:F:45:ARG:HH11	2:F:45:ARG:CG	2.22	0.53
1:G:191:TYR:CE2	1:G:254:GLU:HG2	2.44	0.53
1:C:192:HIS:HE2	2:D:98:ASP:CG	2.12	0.53
1:A:111:ARG:NH1	1:A:128:GLU:HB3	2.24	0.52
1:C:86:ASN:O	2:H:75:LYS:HD3	2.09	0.52
1:C:66:ARG:O	3:Q:4:SER:OG	2.27	0.52
1:E:117:ALA:HB2	2:F:60:TRP:CE2	2.45	0.52
2:B:25:CYS:HB2	2:B:39:LEU:HD21	1.91	0.52
1:C:192:HIS:NE2	2:D:98:ASP:OD1	2.42	0.52
1:A:52:MET:HE1	1:A:171:TYR:CD1	2.45	0.52
1:C:12:VAL:HG22	1:C:94:THR:HG23	1.91	0.51
1:C:226:GLN:H	5:C:302:EDO:H22	1.75	0.51
2:D:3:ARG:NH1	2:D:59:ASP:OD2	2.43	0.51
1:G:244:TRP:CZ2	2:H:99:MET:HE1	2.45	0.51
3:S:3:GLN:NE2	6:S:101:HOH:O	2.40	0.51
1:A:234:ARG:HD2	2:B:10:TYR:CE1	2.46	0.51
1:E:199:VAL:HG11	1:E:254:GLU:HG3	1.93	0.51
2:F:55:SER:HB3	2:F:63:TYR:CZ	2.46	0.51
2:B:3:ARG:HH11	2:B:61:SER:HB3	1.75	0.51
1:G:107:TRP:O	1:G:169:ARG:HD3	2.10	0.51
3:S:4:SER:HB3	6:S:102:HOH:O	2.11	0.51
1:G:230:LEU:HD22	1:G:243:LYS:HE3	1.92	0.50
1:G:70:ASP:HB2	6:G:401:HOH:O	2.10	0.50
1:A:250:PRO:HB2	1:A:253:LYS:HG3	1.93	0.50
1:C:111:ARG:HG2	1:C:113:TYR:CZ	2.46	0.50
2:F:49:VAL:HG22	2:F:68:THR:HB	1.93	0.50
1:A:50:PRO:HA	1:A:53:GLU:OE2	2.11	0.50
1:C:35:ARG:HG2	1:C:36:PHE:N	2.27	0.50
1:G:199:VAL:HG21	1:G:254:GLU:HG3	1.94	0.50
1:A:171:TYR:HA	1:A:174:LEU:HD23	1.93	0.49
2:B:38:ASP:CG	2:B:45:ARG:HD2	2.32	0.49
1:C:243:LYS:N	6:C:402:HOH:O	2.36	0.49
1:C:80:THR:HG23	1:C:83:ARG:HH21	1.77	0.49
2:H:12:ARG:HG2	2:H:13:HIS:ND1	2.28	0.49
1:A:181:ARG:NH2	1:C:186:LYS:HZ2	2.10	0.49
1:C:226:GLN:N	5:C:302:EDO:H22	2.27	0.49
1:G:196:GLN:HG3	1:G:197:VAL:HG22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:GLN:NE2	1:C:89:LYS:HA	2.28	0.49
2:F:45:ARG:HH11	2:F:45:ARG:HG3	1.76	0.49
1:A:19:GLU:HB3	1:A:75:ARG:NH1	2.28	0.49
1:E:180:LEU:HB2	1:G:270:LEU:HD23	1.94	0.49
1:A:5:LEU:O	1:A:100:GLY:HA3	2.12	0.49
1:A:14:ARG:HB2	1:A:17:LEU:HB2	1.95	0.49
1:C:193:PRO:HA	1:C:199:VAL:HG22	1.94	0.49
1:C:255:GLN:O	1:C:273:ARG:NH1	2.46	0.49
1:G:111:ARG:HG2	1:G:113:TYR:CZ	2.46	0.49
1:E:117:ALA:HB2	2:F:60:TRP:CD2	2.48	0.49
1:A:117:ALA:HB2	2:B:60:TRP:CD2	2.48	0.49
1:A:192:HIS:NE2	2:B:98:ASP:HB3	2.28	0.48
1:C:55:GLU:OE2	1:C:170:ARG:NH2	2.38	0.48
1:G:193:PRO:HA	1:G:199:VAL:HG12	1.94	0.48
1:G:35:ARG:NE	2:H:53:ASP:OD1	2.46	0.48
1:A:191:TYR:CE2	1:A:199:VAL:HG21	2.48	0.48
1:C:159:TYR:CE2	1:C:164:CYS:HB2	2.48	0.48
1:E:177:GLU:H	1:E:177:GLU:CD	2.16	0.48
1:A:25:VAL:HB	6:B:108:HOH:O	2.12	0.48
2:H:37:VAL:HG22	2:H:82:VAL:HG22	1.96	0.48
1:C:191:TYR:CE2	1:C:254:GLU:HG2	2.47	0.48
1:G:209:TYR:CD1	1:G:210:PRO:HA	2.48	0.48
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.49	0.48
1:E:260:HIS:HA	1:E:270:LEU:O	2.14	0.48
1:A:13:SER:HA	1:A:20:PRO:HB3	1.94	0.48
1:E:63:GLN:HB2	6:E:364:HOH:O	2.14	0.48
1:E:234:ARG:HD2	2:F:10:TYR:CE1	2.49	0.48
2:B:37:VAL:HG22	2:B:82:VAL:HG22	1.96	0.47
1:C:219:LEU:HD13	1:C:220:ASN:N	2.29	0.47
1:E:152:ASP:OD2	3:R:6:LEU:HB3	2.14	0.47
1:C:234:ARG:HD2	2:D:10:TYR:CE1	2.49	0.47
1:G:75:ARG:O	1:G:79:ARG:HG3	2.14	0.47
1:A:35:ARG:HG2	1:A:36:PHE:N	2.28	0.47
1:E:64:THR:O	1:E:68:LYS:HG3	2.14	0.47
1:A:22:PHE:HE1	1:A:74:PHE:CD2	2.32	0.47
1:G:234:ARG:HD2	2:H:10:TYR:CE1	2.50	0.47
1:C:41:ASP:OD1	1:C:41:ASP:N	2.47	0.47
1:E:219:LEU:HD23	1:E:257:TYR:CD2	2.49	0.47
1:G:203:CYS:O	1:G:244:TRP:HA	2.14	0.47
1:G:226:GLN:C	1:G:228:MET:N	2.68	0.47
2:B:3:ARG:NH1	2:B:61:SER:HB3	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:17:ASN:HA	2:H:72:PRO:O	2.15	0.47
1:G:111:ARG:HG3	1:G:112:GLY:N	2.29	0.47
2:F:6:LYS:HE3	2:F:28:SER:OG	2.15	0.47
2:F:41:LYS:HB2	2:F:46:ILE:HD11	1.97	0.47
1:A:32:GLN:NE2	1:A:48:ARG:HG3	2.31	0.46
1:A:103:VAL:HB	1:A:107:TRP:HA	1.96	0.46
1:C:257:TYR:O	1:C:273:ARG:HG3	2.16	0.46
1:G:54:GLN:O	1:G:54:GLN:HG2	2.15	0.46
1:G:133:TRP:HB2	1:G:144:ARG:HG3	1.98	0.46
1:E:157:ARG:HH21	1:E:157:ARG:HB2	1.81	0.46
2:F:6:LYS:NZ	2:F:8:GLN:HE21	2.13	0.46
1:A:111:ARG:HG3	1:A:112:GLY:N	2.30	0.46
2:D:50:GLU:HB2	2:D:67:TYR:CZ	2.50	0.46
1:G:5:LEU:HB2	1:G:168:LEU:HD13	1.97	0.46
1:E:6:ARG:HH21	1:E:6:ARG:HG3	1.80	0.46
1:G:21:ARG:CZ	1:G:23:ILE:HD11	2.46	0.46
1:C:35:ARG:HD3	2:D:53:ASP:OD2	2.15	0.46
2:D:51:HIS:HB3	2:D:66:TYR:CD2	2.50	0.46
2:D:81:ARG:HG3	2:D:92:ILE:HG13	1.97	0.46
2:F:1:ILE:HD13	2:F:3:ARG:NH1	2.31	0.46
2:F:45:ARG:CG	2:F:45:ARG:NH1	2.79	0.46
1:A:6:ARG:NH1	1:A:102:ASP:OD1	2.37	0.46
1:A:129:ASP:O	1:A:131:LYS:HD2	2.16	0.46
1:E:219:LEU:HD23	1:E:257:TYR:CG	2.51	0.46
2:H:12:ARG:HG2	2:H:13:HIS:CE1	2.51	0.45
2:B:50:GLU:HB2	2:B:67:TYR:CZ	2.51	0.45
2:B:36:GLU:OE2	2:B:83:ASN:HB3	2.17	0.45
1:A:259:CYS:HB3	6:A:403:HOH:O	2.17	0.45
1:G:55:GLU:HG2	1:G:59:TYR:CD2	2.52	0.45
2:B:24:ASN:HB3	2:B:65:LEU:HD11	1.99	0.45
1:C:5:LEU:O	1:C:100:GLY:HA3	2.16	0.45
1:E:97:ARG:HH21	1:E:114:HIS:CD2	2.34	0.45
2:F:51:HIS:HA	2:F:65:LEU:O	2.17	0.45
1:E:14:ARG:CZ	1:E:21:ARG:HB2	2.47	0.45
1:E:47:PRO:HG3	1:E:60:TRP:CZ2	2.51	0.45
1:G:177:GLU:CD	1:G:177:GLU:H	2.21	0.45
2:D:70:PHE:HD2	2:D:78:TYR:CZ	2.35	0.45
1:G:183:ASP:HB2	1:G:209:TYR:H	1.82	0.45
1:A:21:ARG:NH1	1:A:39:ASP:OD2	2.46	0.44
1:G:103:VAL:HG11	1:G:165:VAL:HG13	1.99	0.44
1:G:4:SER:HB2	1:G:6:ARG:NH2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:260:HIS:HA	1:G:270:LEU:O	2.17	0.44
1:C:192:HIS:NE2	2:D:98:ASP:CG	2.70	0.44
1:E:219:LEU:HD22	1:E:256:ASN:O	2.18	0.44
1:A:62:GLU:HG2	3:P:1:TYR:OH	2.18	0.44
2:B:6:LYS:O	2:B:27:VAL:HA	2.18	0.44
1:G:218:GLN:HE21	1:G:224:LEU:CD2	2.29	0.44
2:H:58:LYS:HD3	2:H:58:LYS:H	1.81	0.44
1:A:209:TYR:CG	1:A:210:PRO:HA	2.52	0.44
1:C:37:ASP:N	6:C:420:HOH:O	2.48	0.44
2:H:36:GLU:O	2:H:82:VAL:HA	2.18	0.44
1:C:159:TYR:CZ	1:C:164:CYS:HB2	2.52	0.44
1:E:261:VAL:HB	1:E:270:LEU:HB2	2.00	0.44
2:F:31:HIS:CE1	6:F:203:HOH:O	2.70	0.44
1:E:160:LEU:O	1:E:165:VAL:HG23	2.17	0.44
1:G:42:ASN:HB3	1:G:44:ARG:NH1	2.33	0.44
1:A:232:GLU:OE1	2:B:6:LYS:HD2	2.18	0.43
1:C:167:TRP:CG	3:Q:1:TYR:HB2	2.52	0.43
1:A:231:VAL:O	1:A:243:LYS:HE2	2.18	0.43
1:E:228:MET:HE3	1:E:230:LEU:HD13	1.99	0.43
1:C:22:PHE:HE1	1:C:74:PHE:CD2	2.36	0.43
1:E:71:GLU:O	1:E:75:ARG:HG3	2.18	0.43
1:A:51:TRP:CZ2	1:A:179:LEU:HD21	2.52	0.43
1:A:104:GLY:O	1:A:107:TRP:HD1	2.01	0.43
1:A:187:ALA:HA	1:A:204:TRP:O	2.19	0.43
1:C:103:VAL:HB	1:C:107:TRP:HA	2.00	0.43
1:A:226:GLN:CD	1:A:226:GLN:H	2.22	0.43
1:C:111:ARG:HD2	1:C:128:GLU:OE2	2.19	0.43
1:E:82:GLN:NE2	1:E:89:LYS:HA	2.33	0.43
1:G:23:ILE:HD13	2:H:54:LEU:HB3	2.00	0.43
1:G:117:ALA:HB2	2:H:60:TRP:CE2	2.52	0.43
1:A:199:VAL:O	1:A:248:VAL:HA	2.18	0.43
1:A:272:LEU:CD2	1:C:177:GLU:HG3	2.49	0.43
1:G:22:PHE:HE1	1:G:74:PHE:CD2	2.37	0.43
1:E:232:GLU:HB3	2:F:6:LYS:NZ	2.34	0.43
1:G:5:LEU:O	1:G:100:GLY:HA3	2.19	0.43
1:A:191:TYR:CD2	1:A:199:VAL:HG21	2.54	0.42
1:C:109:LEU:HB2	1:C:165:VAL:HG21	2.01	0.42
1:C:191:TYR:CZ	1:C:199:VAL:HG21	2.54	0.42
1:E:228:MET:CE	1:E:230:LEU:HD13	2.49	0.42
2:F:24:ASN:HB3	2:F:65:LEU:HD11	2.00	0.42
1:G:70:ASP:OD2	1:G:97:ARG:NH1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:45:PHE:CE2	1:G:67:ALA:HB2	2.54	0.42
1:A:2:PRO:HA	1:A:103:VAL:O	2.18	0.42
2:B:51:HIS:HB3	2:B:66:TYR:CD2	2.54	0.42
1:C:254:GLU:H	1:C:254:GLU:CD	2.21	0.42
2:H:6:LYS:O	2:H:27:VAL:HA	2.19	0.42
1:E:254:GLU:H	1:E:254:GLU:CD	2.21	0.42
1:G:209:TYR:CG	1:G:210:PRO:HA	2.54	0.42
6:A:418:HOH:O	2:B:53:ASP:HB2	2.20	0.42
1:E:146:LYS:HE2	3:R:8:ILE:O	2.20	0.42
1:E:270:LEU:HD23	1:G:180:LEU:HB2	2.02	0.42
1:A:183:ASP:OD2	6:A:402:HOH:O	2.21	0.42
1:C:114:HIS:CD2	6:C:441:HOH:O	2.71	0.42
1:A:64:THR:O	1:A:68:LYS:HG3	2.20	0.42
1:C:220:ASN:C	1:C:222:GLU:N	2.72	0.42
1:E:238:ASP:OD2	6:E:304:HOH:O	2.21	0.42
1:A:170:ARG:NH1	1:A:173:GLU:OE1	2.53	0.42
1:A:45:PHE:CE2	1:A:67:ALA:HB2	2.55	0.41
1:A:234:ARG:CG	1:A:242:GLN:HB2	2.49	0.41
2:B:11:SER:OG	2:B:13:HIS:O	2.29	0.41
1:A:192:HIS:O	1:A:199:VAL:HG23	2.21	0.41
1:C:14:ARG:HB2	1:C:17:LEU:HB2	2.02	0.41
1:C:35:ARG:HD3	2:D:53:ASP:CG	2.41	0.41
1:E:35:ARG:O	1:E:35:ARG:HG3	2.19	0.41
1:G:264:LYS:HE2	6:G:417:HOH:O	2.20	0.41
1:A:119:ASP:HB3	2:B:0:MET:HA	2.03	0.41
1:A:130:LEU:HD22	1:A:160:LEU:HD13	2.01	0.41
1:G:191:TYR:CD2	1:G:254:GLU:HG2	2.55	0.41
1:A:54:GLN:CD	1:A:54:GLN:H	2.24	0.41
1:A:260:HIS:HD2	6:A:460:HOH:O	2.04	0.41
1:E:97:ARG:HE	1:E:114:HIS:CD2	2.39	0.41
1:A:75:ARG:HH11	1:A:75:ARG:HD3	1.68	0.41
1:A:167:TRP:CG	3:P:1:TYR:HB2	2.56	0.41
1:E:209:TYR:CG	1:E:210:PRO:HA	2.55	0.41
1:G:155:TYR:CD2	3:S:6:LEU:HB2	2.56	0.41
1:G:230:LEU:HD23	1:G:230:LEU:HA	1.94	0.41
1:C:208:PHE:CE1	1:C:241:PHE:HB2	2.56	0.41
1:E:224:LEU:HA	1:E:224:LEU:HD23	1.75	0.41
2:B:48:LYS:HB3	2:B:48:LYS:HE3	1.96	0.40
1:A:129:ASP:HB2	1:A:131:LYS:HD2	2.02	0.40
1:C:260:HIS:HA	1:C:270:LEU:O	2.21	0.40
2:F:26:TYR:CZ	2:F:28:SER:HB3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:6:LYS:O	2:D:27:VAL:HA	2.21	0.40
1:E:144:ARG:HD3	6:E:332:HOH:O	2.22	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:409:HOH:O	6:E:328:HOH:O[1_656]	2.01	0.19
6:C:425:HOH:O	6:G:469:HOH:O[1_645]	2.10	0.10
6:A:453:HOH:O	6:E:324:HOH:O[1_646]	2.11	0.09
1:A:111:ARG:NH1	2:B:47:GLU:OE1[1_655]	2.15	0.05
1:E:128:GLU:OE1	2:F:48:LYS:N[1_455]	2.16	0.04

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	271/275 (98%)	265 (98%)	5 (2%)	1 (0%)	34	42
1	C	271/275 (98%)	262 (97%)	5 (2%)	4 (2%)	10	10
1	E	271/275 (98%)	262 (97%)	8 (3%)	1 (0%)	34	42
1	G	271/275 (98%)	263 (97%)	5 (2%)	3 (1%)	14	15
2	B	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
2	D	98/100 (98%)	97 (99%)	0	1 (1%)	15	17
2	F	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
2	H	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
3	P	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	Q	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	R	7/9 (78%)	6 (86%)	1 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	S	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
All	All	1504/1536 (98%)	1463 (97%)	31 (2%)	10 (1%)	22	26

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	ASP
1	C	220	ASN
1	E	41	ASP
1	G	221	GLY
1	G	227	ASP
1	C	196	GLN
1	C	221	GLY
1	G	195	SER
1	C	195	SER
2	D	48	LYS

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	229/235 (97%)	221 (96%)	8 (4%)	36	50
1	C	231/235 (98%)	225 (97%)	6 (3%)	46	63
1	E	231/235 (98%)	226 (98%)	5 (2%)	52	69
1	G	231/235 (98%)	221 (96%)	10 (4%)	29	40
2	B	94/95 (99%)	90 (96%)	4 (4%)	29	40
2	D	94/95 (99%)	89 (95%)	5 (5%)	22	31
2	F	94/95 (99%)	91 (97%)	3 (3%)	39	54
2	H	95/95 (100%)	92 (97%)	3 (3%)	39	54
3	P	8/8 (100%)	8 (100%)	0	100	100
3	Q	8/8 (100%)	7 (88%)	1 (12%)	4	5
3	R	8/8 (100%)	8 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	S	8/8 (100%)	8 (100%)	0	100	100
All	All	1331/1352 (98%)	1286 (97%)	45 (3%)	37	51

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ARG
1	A	35	ARG
1	A	70	ASP
1	A	88	SER
1	A	95	PHE
1	A	216	THR
1	A	226	GLN
1	A	264	LYS
2	B	0	MET
2	B	58	LYS
2	B	70	PHE
2	B	98	ASP
1	C	45	PHE
1	C	70	ASP
1	C	95	PHE
1	C	115	GLN
1	C	196	GLN
1	C	199	VAL
2	D	19	LYS
2	D	45	ARG
2	D	48	LYS
2	D	65	LEU
2	D	70	PHE
3	Q	6	LEU
1	E	14	ARG
1	E	70	ASP
1	E	95	PHE
1	E	226	GLN
1	E	251	LEU
2	F	6	LYS
2	F	27	VAL
2	F	70	PHE
1	G	35	ARG
1	G	45	PHE
1	G	54	GLN
1	G	70	ASP

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Mol	Chain	Res	Type
1	G	95	PHE
1	G	108	ARG
1	G	194	ARG
1	G	225	THR
1	G	228	MET
1	G	272	LEU
2	H	45	ARG
2	H	58	LYS
2	H	70	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	HIS
1	A	260	HIS
1	C	54	GLN
1	C	72	GLN
1	C	115	GLN
1	E	72	GLN
1	E	82	GLN
1	E	86	ASN
1	E	149	GLN
2	F	8	GLN
1	G	114	HIS
1	G	218	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

9 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	EDO	A	303	-	3,3,3	0.47	0	2,2,2	0.37	0
4	GOL	G	301	-	5,5,5	0.34	0	5,5,5	0.54	0
4	GOL	F	101	-	5,5,5	0.38	0	5,5,5	0.19	0
4	GOL	H	101	-	5,5,5	0.34	0	5,5,5	0.34	0
5	EDO	C	301	-	3,3,3	0.48	0	2,2,2	0.35	0
5	EDO	C	302	-	3,3,3	0.41	0	2,2,2	0.30	0
4	GOL	A	301	-	5,5,5	0.35	0	5,5,5	0.35	0
4	GOL	A	302	-	5,5,5	0.36	0	5,5,5	0.20	0
4	GOL	D	101	-	5,5,5	0.42	0	5,5,5	0.40	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	303	-	-	1/1/1/1	-
4	GOL	G	301	-	-	4/4/4/4	-
4	GOL	F	101	-	-	4/4/4/4	-
4	GOL	H	101	-	-	2/4/4/4	-
5	EDO	C	301	-	-	0/1/1/1	-
5	EDO	C	302	-	-	0/1/1/1	-
4	GOL	A	301	-	-	4/4/4/4	-
4	GOL	A	302	-	-	2/4/4/4	-
4	GOL	D	101	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	301	GOL	O1-C1-C2-C3
4	A	301	GOL	C1-C2-C3-O3
4	D	101	GOL	O1-C1-C2-C3
4	F	101	GOL	O1-C1-C2-O2
4	F	101	GOL	C1-C2-C3-O3
4	G	301	GOL	O1-C1-C2-C3
4	G	301	GOL	C1-C2-C3-O3
4	G	301	GOL	O2-C2-C3-O3
4	A	301	GOL	O2-C2-C3-O3
4	H	101	GOL	O1-C1-C2-O2
4	A	302	GOL	O1-C1-C2-C3
4	F	101	GOL	O1-C1-C2-C3
4	H	101	GOL	O1-C1-C2-C3
4	A	301	GOL	O1-C1-C2-O2
4	D	101	GOL	O1-C1-C2-O2
4	F	101	GOL	O2-C2-C3-O3
4	G	301	GOL	O1-C1-C2-O2
4	D	101	GOL	C1-C2-C3-O3
4	A	302	GOL	O1-C1-C2-O2
5	A	303	EDO	O1-C1-C2-O2
4	D	101	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	302	EDO	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	273/275 (99%)	-0.64	0 100 100	12, 24, 40, 53	0
1	C	273/275 (99%)	-0.69	0 100 100	10, 23, 39, 59	0
1	E	273/275 (99%)	-0.63	1 (0%) 92 95	11, 24, 42, 58	0
1	G	273/275 (99%)	-0.61	2 (0%) 87 91	12, 23, 38, 62	2 (0%)
2	B	100/100 (100%)	-0.69	0 100 100	14, 30, 46, 55	0
2	D	100/100 (100%)	-0.61	0 100 100	14, 28, 49, 58	0
2	F	100/100 (100%)	-0.70	0 100 100	16, 29, 44, 50	0
2	H	100/100 (100%)	-0.61	0 100 100	16, 33, 48, 54	0
3	P	9/9 (100%)	-0.57	0 100 100	16, 17, 30, 31	0
3	Q	9/9 (100%)	-0.76	0 100 100	11, 16, 18, 19	0
3	R	9/9 (100%)	-0.70	0 100 100	16, 19, 24, 28	0
3	S	9/9 (100%)	-0.61	0 100 100	16, 21, 23, 31	0
All	All	1528/1536 (99%)	-0.65	3 (0%) 95 96	10, 25, 44, 62	2 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	221	GLY	4.8
1	E	196	GLN	2.9
1	G	222	GLU	2.4

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	GOL	F	101	6/6	0.94	0.10	15,24,28,37	0
4	GOL	G	301	6/6	0.96	0.12	10,26,34,36	0
4	GOL	A	301	6/6	0.97	0.08	16,23,24,29	0
4	GOL	A	302	6/6	0.97	0.10	26,27,35,38	0
4	GOL	H	101	6/6	0.98	0.09	21,28,35,36	0
5	EDO	C	302	4/4	0.98	0.09	11,18,23,27	0
5	EDO	A	303	4/4	0.99	0.07	20,21,21,29	0
5	EDO	C	301	4/4	0.99	0.05	13,17,20,23	0
4	GOL	D	101	6/6	0.99	0.07	10,25,40,46	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.